

6.730 Physics for Solid State Applications

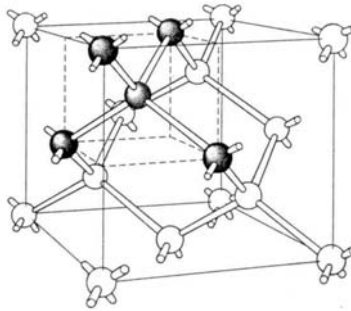
Lecture 10 & 11: Lattice Waves in 2D and 3D

Outline

- Algebra for Bond Stretching in 3-D
- Example: 2-D Lattice Waves with Bond Stretching
- Algebra for Bond Bending in 3-D
- Example: 1-D and 2-D Lattice Waves with Bond Stretching and Bending
- 3-D Examples

February 25 and 27, 2004

Lattice Waves in 3-D Crystals



Displacements of basis atoms along three directions...

$$\begin{array}{ll} u_{1x}[\mathbf{R}_n] & u_{2x}[\mathbf{R}_n] \\ u_{1y}[\mathbf{R}_n] & u_{2y}[\mathbf{R}_n] \\ u_{1z}[\mathbf{R}_n] & u_{2z}[\mathbf{R}_n] \end{array}$$

Lattice Waves in 3-D Crystals

Second order Taylor series expansion for total potential energy:

$$V(\{u[\mathbf{R}_s, t]\}) = V_0 + \frac{1}{2} \sum_i \sum_j \sum_{\mathbf{R}_p} \sum_{\mathbf{R}_m} u_i[\mathbf{R}_p, t] \tilde{D}_{i,j}(\mathbf{R}_p, \mathbf{R}_m) u_j[\mathbf{R}_m, t]$$

Harmonic Matrix:

$$\tilde{D}_{i,j}(\mathbf{R}_p, \mathbf{R}_m) = \left(\frac{\partial^2 V}{\partial u_i[\mathbf{R}_p, t] \partial u_j[\mathbf{R}_m, t]} \right)_{\text{eq}}$$

Equation of motion for lattice atoms assuming 'plane wave' solutions:

$$(\mathbf{M}^{-1} \mathbf{D}(\mathbf{k})) \vec{\epsilon} = \omega^2 \vec{\epsilon}$$

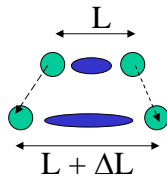
Dynamical Matrix:

$$D_{i,j}(\mathbf{k}) = \sum_{\mathbf{R}_p} \left(\frac{\partial^2 V}{\partial u_i[\mathbf{R}_s + \mathbf{R}_p, t] \partial u_j[\mathbf{R}_s, t]} \right)_{\text{eq}} e^{-i\mathbf{k} \cdot \mathbf{R}_p}$$

Lattice Waves in 3-D Crystals

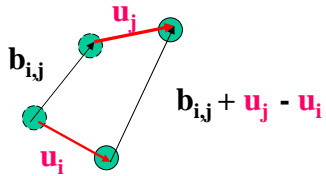
$$(\mathbf{M}^{-1} \mathbf{D}(\mathbf{k})) \vec{\epsilon} = \omega^2 \vec{\epsilon}$$

$$\epsilon[\mathbf{R}_n] = \begin{pmatrix} \epsilon_{1x}[\mathbf{R}_n] \\ \epsilon_{2x}[\mathbf{R}_n] \\ \vdots \\ \epsilon_{1y}[\mathbf{R}_n] \\ \epsilon_{2y}[\mathbf{R}_n] \\ \vdots \\ \epsilon_{1z}[\mathbf{R}_n] \\ \epsilon_{2z}[\mathbf{R}_n] \\ \vdots \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} M_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & M_2 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & M_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & M_2 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & M_1 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & M_2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



Bond Stretching

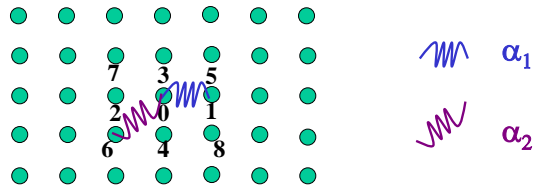
$$E_s = \frac{1}{2} \alpha_s (\Delta L)^2$$



$$\Delta L = |b + u_j - u_i| - |b| \quad \longrightarrow \quad \Delta L \approx \hat{b}_{i,j} \cdot (u_j - u_i)$$

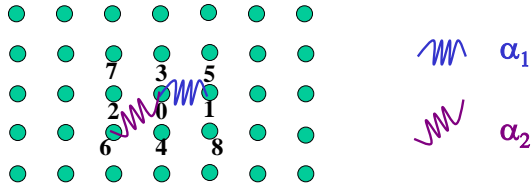
$$E_s = \frac{1}{2} \alpha_s \left(\hat{b}_{i,j} \cdot (u_j - u_i) \right)^2$$

Example: 2-D Lattice with Bond Stretching



$$\begin{aligned} V = & \dots + \frac{\alpha_1}{2} |\hat{a}_1 \cdot (u[\mathbf{R} + \mathbf{a}_1] - u[\mathbf{R}])|^2 + \frac{\alpha_1}{2} |\hat{a}_1 \cdot (u[\mathbf{R} - \mathbf{a}_1] - u[\mathbf{R}])|^2 \\ & + \frac{\alpha_1}{2} |\hat{a}_2 \cdot (u[\mathbf{R} + \mathbf{a}_2] - u[\mathbf{R}])|^2 + \frac{\alpha_1}{2} |\hat{a}_2 \cdot (u[\mathbf{R} - \mathbf{a}_2] - u[\mathbf{R}])|^2 \\ & + \frac{\alpha_2}{2} \left| \frac{\hat{a}_1 + \hat{a}_2}{\sqrt{2}} \cdot (u[\mathbf{R} + \mathbf{a}_1 + \mathbf{a}_2] - u[\mathbf{R}]) \right|^2 \\ & + \frac{\alpha_2}{2} \left| \frac{-\hat{a}_1 + \hat{a}_2}{\sqrt{2}} \cdot (u[\mathbf{R} - \mathbf{a}_1 + \mathbf{a}_2] - u[\mathbf{R}]) \right|^2 \\ & + \frac{\alpha_2}{2} \left| \frac{\hat{a}_1 - \hat{a}_2}{\sqrt{2}} \cdot (u[\mathbf{R} + \mathbf{a}_1 - \mathbf{a}_2] - u[\mathbf{R}]) \right|^2 + \dots \end{aligned}$$

Example: 2-D Lattice with Bond Stretching
Elements of the Dynamical Matrix



$$\begin{aligned}
 D_{xx}(\mathbf{k}) &= \alpha_1 (1 - e^{-i\mathbf{k}\cdot\mathbf{a}_1}) + \alpha_1 (1 - e^{i\mathbf{k}\cdot\mathbf{a}_1}) + 0 + 0 \\
 &+ \frac{\alpha_2}{2} (1 - e^{-i\mathbf{k}\cdot(\mathbf{a}_1+\mathbf{a}_2)}) + \frac{\alpha_2}{2} (1 - e^{-i\mathbf{k}\cdot(-\mathbf{a}_1-\mathbf{a}_2)}) \\
 &+ \frac{\alpha_2}{2} (1 - e^{-i\mathbf{k}\cdot(-\mathbf{a}_1+\mathbf{a}_2)}) + \frac{\alpha_2}{2} (1 - e^{-i\mathbf{k}\cdot(\mathbf{a}_1-\mathbf{a}_2)})
 \end{aligned}$$

Example: 2-D Lattice with Bond Stretching
Dynamical Matrix

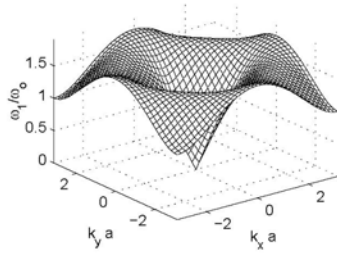
$$D(\mathbf{k}) = \begin{pmatrix} 2\alpha_1(1 - \cos k_x a) + 2\alpha_2(1 - \cos k_x a \cos k_y a) & 2\alpha_2 \sin k_x a \sin k_y a \\ 2\alpha_2 \sin k_x a \sin k_y a & 2\alpha_1(1 - \cos k_y a) + 2\alpha_2(1 - \cos k_x a \cos k_y a) \end{pmatrix}$$

$$\mathbf{M} = \mathbf{M} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

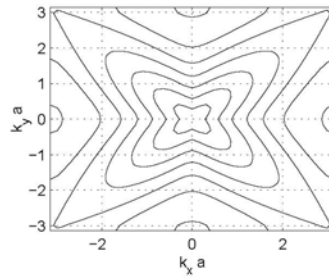
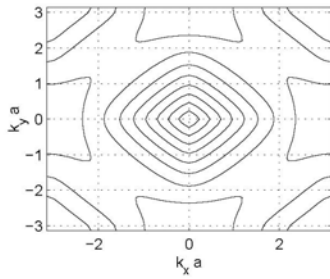
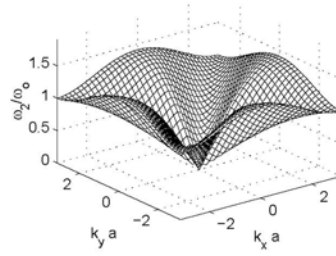
$$\frac{1}{M} \mathbf{D}(\mathbf{k}) \tilde{\epsilon} = \omega^2 \tilde{\epsilon}$$

2d Dispersion Relation

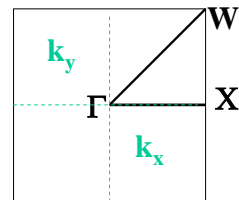
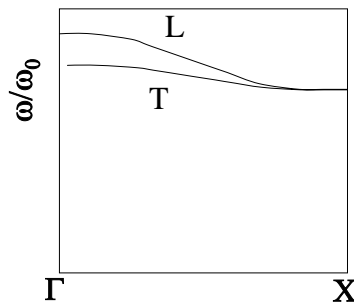
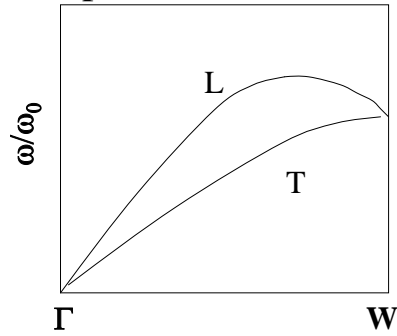
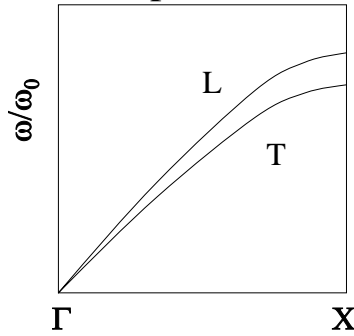
Longitudinal Mode for $\alpha_2/\alpha_1 = 0.5$



Transverse Mode for $\alpha_2/\alpha_1 = 0.5$



Dispersion Relation on special directions



Example: 2-D Lattice with Bond Stretching Dispersion Relation

$$D(k_x, 0) = \begin{pmatrix} 2(\alpha_1 + \alpha_2)(1 - \cos k_x a) & 0 \\ 0 & 2\alpha_2(1 - \cos k_x a) \end{pmatrix}$$

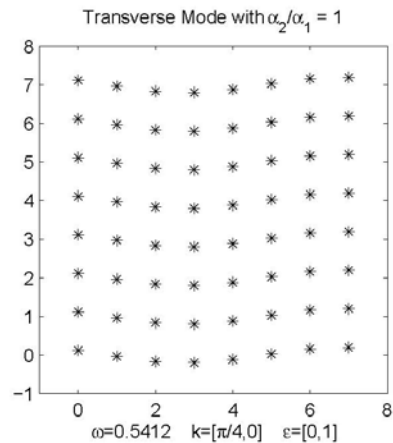
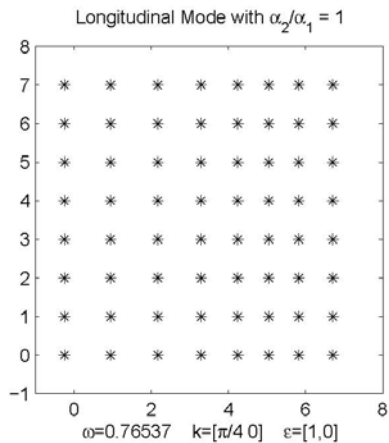
$$\omega_1(k_x, 0) = \sqrt{\frac{4(\alpha_1 + \alpha_2)}{M}} \sin \frac{k_x a}{2} \quad \vec{e}_1(k_x, 0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\omega_2(k_x, 0) = \sqrt{\frac{4\alpha_2}{M}} \sin \frac{k_x a}{2} \quad \vec{e}_2(k_x, 0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\tilde{u}_i[\mathbf{R}_n, t] = e^{i(\mathbf{k} \cdot \mathbf{R}_n - \omega_i(\mathbf{k})t)} \tilde{e}_i(\mathbf{k})$$

2D Modes

$$D(\mathbf{k}) = \begin{pmatrix} 4\alpha_{sA} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_1}{2} + 4\alpha_{\phi B} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_2}{2} & 0 \\ 0 & 4\alpha_{sB} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_2}{2} + 4\alpha_{\phi A} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_1}{2} \end{pmatrix}$$



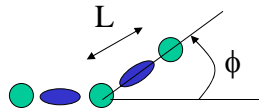
Example: 2-D Lattice with Bond Stretching
 Relating Microscopic and Macroscopic Models

$$\omega_1(k_x, 0) \approx \underbrace{\sqrt{\frac{(\alpha_1 + \alpha_2)a^2}{M}}}_{c_L} k_x \quad \text{and} \quad \omega_2(k_x, 0) \approx \underbrace{\sqrt{\frac{\alpha_2 a^2}{M}}}_{c_T} k_x$$

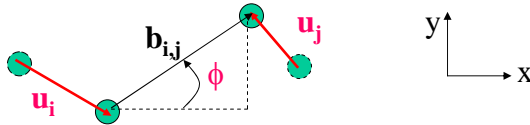
$$c_L = \sqrt{(\lambda + 2\mu)/\rho} \quad \text{and} \quad c_T = \sqrt{\mu/\rho}$$

$$\mu = \alpha_2 \quad \text{and} \quad \lambda = \alpha_1 - \alpha_2$$

Bond Bending



$$E_\phi = \frac{1}{2} \alpha_\phi L^2 (\Delta\phi)^2$$

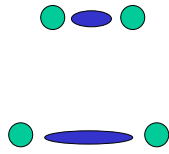


$$\tan(\Delta\phi) = \frac{u_{jy} - u_{iy}}{L + \Delta L} \quad \longrightarrow \quad (\Delta\phi) = \frac{u_{jy} - u_{iy}}{L}$$

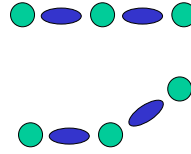
$$u_{iy} = u_i - \hat{b}_{i,j} (\hat{b}_{i,j} \cdot u_i) \quad L^2 (\Delta\phi)^2 = |u_{iy} - u_{jy}|^2$$

$$E_\phi = \frac{1}{2} \alpha_\phi \left(|u_i - u_j|^2 - [\hat{b}_{i,j} \cdot (u_i - u_j)]^2 \right)$$

Bond Stretching and Bending



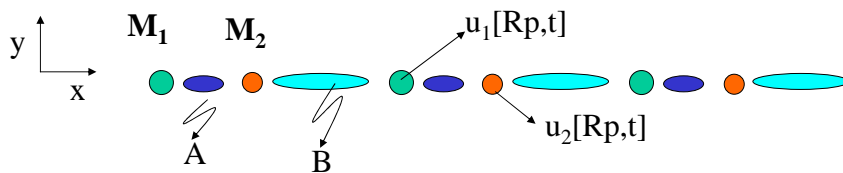
$$E_s = \frac{1}{2} \alpha_s (\Delta L)^2$$



$$E_\phi = \frac{1}{2} \alpha_\phi L^2 (\Delta\phi)^2$$

$$E_s = \frac{1}{2} \alpha_s (\hat{\mathbf{b}}_{i,j} \cdot (\mathbf{u}_j - \mathbf{u}_i))^2 \quad E_\phi = \frac{1}{2} \alpha_\phi (|\mathbf{u}_i - \mathbf{u}_j|^2 - [\hat{\mathbf{b}}_{i,j} \cdot (\mathbf{u}_i - \mathbf{u}_j)]^2)$$

Example: 1-D Diatomic Lattice with Bond Stretching and Bending Potential Energy



$$E_s = \frac{1}{2} \alpha_s (\Delta L)^2$$

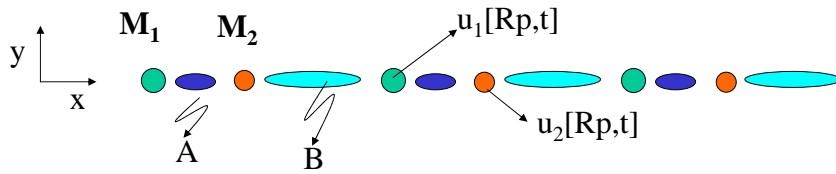
$$E_\phi = \frac{1}{2} \alpha_\phi L^2 (\Delta\phi)^2$$

$$E_s = \frac{1}{2} \alpha_s (\hat{\mathbf{b}}_{i,j} \cdot (\mathbf{u}_j - \mathbf{u}_i))^2 \quad E_\phi = \frac{1}{2} \alpha_\phi (|\mathbf{u}_i - \mathbf{u}_j|^2 - [\hat{\mathbf{b}}_{i,j} \cdot (\mathbf{u}_i - \mathbf{u}_j)]^2)$$

$$E_s = \frac{1}{2} \alpha_{sA} (u_{1x}[\mathbf{R}] - u_{2x}[\mathbf{R}])^2$$

$$E_\phi = \frac{1}{2} \alpha_\phi |u_{1y} - u_{2y}|^2$$

Example: '1-D' Diatomic Lattice with Bond Stretching and Bending
Potential Energy

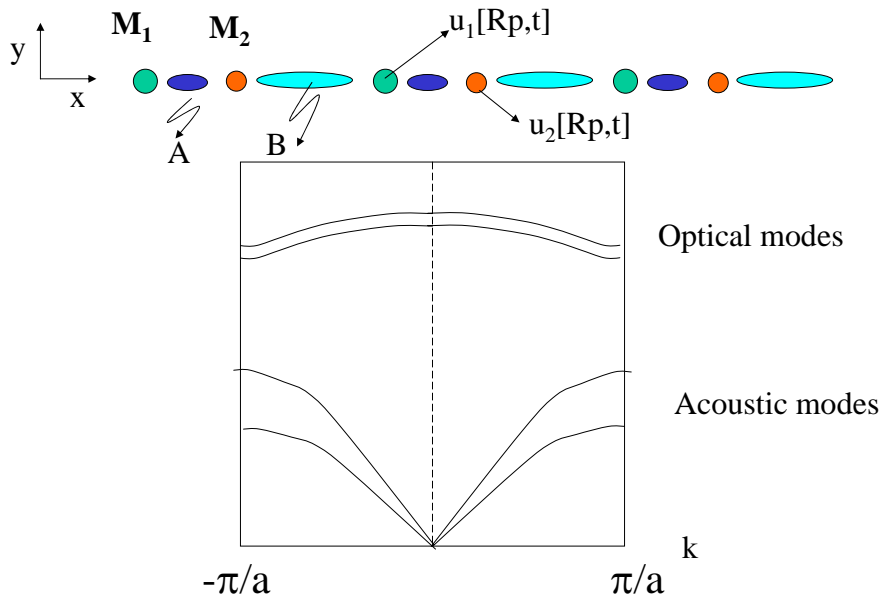


$$V = \dots \frac{1}{2} \alpha_{sA} (u_{1x}[\mathbf{R}] - u_{2x}[\mathbf{R}])^2 + \frac{1}{2} \alpha_{\phi A} (u_{1y}[\mathbf{R}] - u_{2y}[\mathbf{R}])^2$$

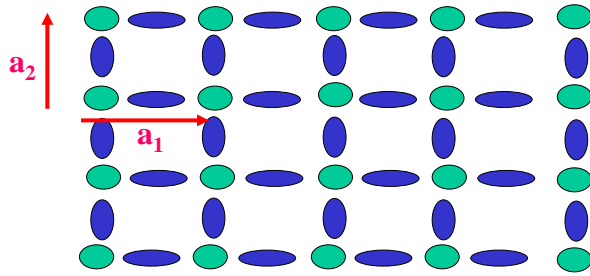
$$+ \frac{1}{2} \alpha_{sB} (u_{1x}[\mathbf{R}] - u_{2x}[\mathbf{R} - \mathbf{a}])^2 + \frac{1}{2} \alpha_{\phi B} (u_{1y}[\mathbf{R}] - u_{2y}[\mathbf{R} - \mathbf{a}])^2 + \dots$$

$$\mathbf{D}(\mathbf{k}) = \begin{pmatrix} u_{1x} & u_{2x} & u_{1y} & u_{2y} \\ u_{1x} & \alpha_{sA} + \alpha_{sB} & -\alpha_{sA} - \alpha_{sB}e^{-ika} & 0 & 0 & 0 \\ u_{2x} & -\alpha_{sA} - \alpha_{sB}e^{ika} & \alpha_{sA} + \alpha_{sB} & 0 & 0 & 0 \\ u_{1y} & 0 & 0 & \alpha_{\phi A} + \alpha_{\phi B} & -\alpha_{\phi A} - \alpha_{\phi B}e^{-ika} & \\ u_{2y} & 0 & 0 & -\alpha_{\phi A} - \alpha_{\phi B}e^{ika} & \alpha_{\phi A} + \alpha_{\phi B} & \end{pmatrix}$$

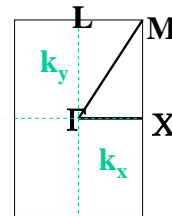
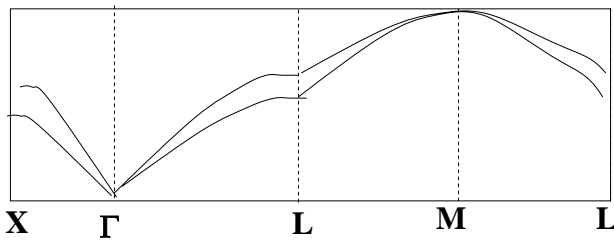
1-D Diatomic Lattice with Bond Stretching and Bending
Dispersion Relation



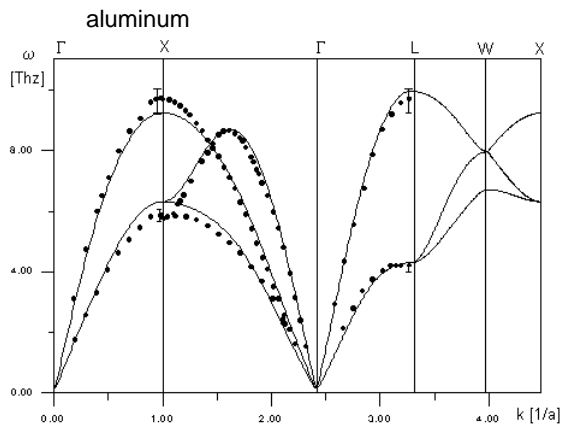
2d rectangular monatomic crystal



$$D(\mathbf{k}) = \begin{pmatrix} 4\alpha_{sA} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_1}{2} + 4\alpha_{\phi B} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_2}{2} & 0 \\ 0 & 4\alpha_{sB} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_2}{2} + 4\alpha_{\phi A} \sin^2 \frac{\mathbf{k} \cdot \mathbf{a}_1}{2} \end{pmatrix}$$

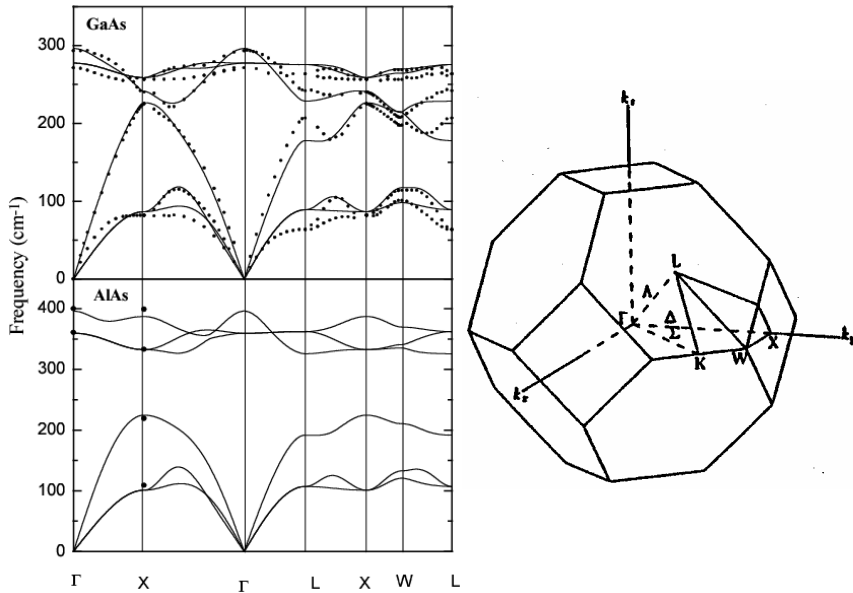


Phonon Dispersion in 3D Cubic Crystal



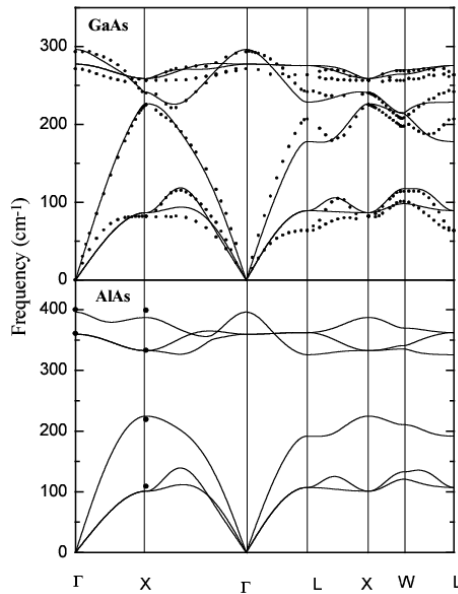
<http://debian.mps.krakow.pl/phonon/Public/phrefer.html>

Phonon Dispersion in FCC with 2 Atom Basis



<http://debian.mps.krakow.pl/phonon/Public/phrefer.html>

Phonon Dispersion in FCC with 2 Atom Basis



<http://debian.mps.krakow.pl/phonon/Public/phrefer.html>